



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 08:06 AM EDT

PDB ID : 1TKD  
Title : T7 DNA polymerase ternary complex with 8 oxo guanosine and dCMP at the elongation site  
Authors : Brieba, L.G.; Eichman, B.F.; Kokoska, R.J.; Doublet, S.; Kunkel, T.A.; Ellenberger, T.  
Deposited on : 2004-06-08  
Resolution : 2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

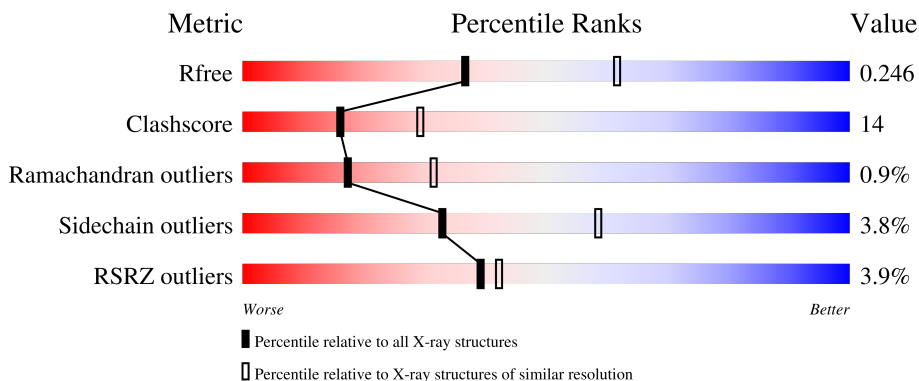
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	P	22	
2	T	26	
3	A	698	
4	B	108	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7842 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*AP\*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	16	325	153	63	93	16	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*CP\*CP\*AP\*(8OG)P\*TP\*GP\*GP\*CP\*AP\*CP\*TP\*GP\*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	19	391	184	71	117	19	0	0	0

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	698	5534	3520	960	1030	24	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P00581
A	?	-	ARG	deletion	UNP P00581
A	?	-	PHE	deletion	UNP P00581
A	?	-	GLY	deletion	UNP P00581
A	?	-	SER	deletion	UNP P00581
A	?	-	HIS	deletion	UNP P00581

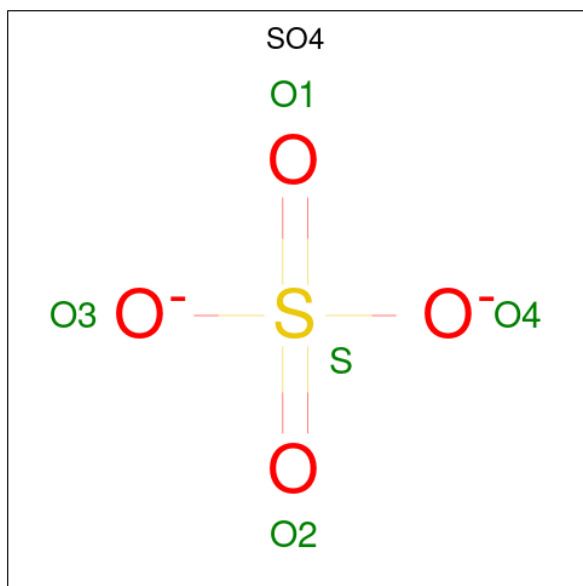
- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	105	802	518	129	152	3	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

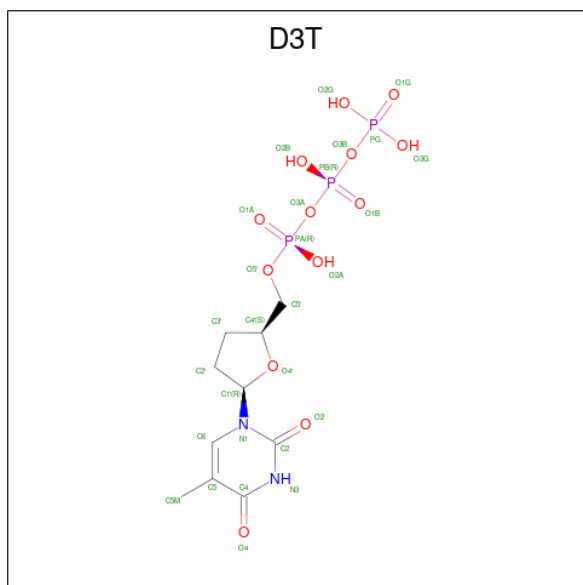
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Mg 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



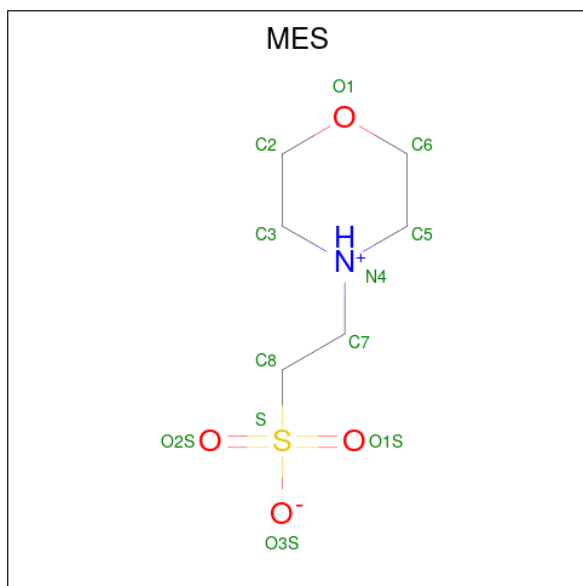
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is 2',3'-DIDEOXY-THYMIDINE-5'-TRIPHOSPHATE (three-letter code: D3T) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>2</sub>O<sub>13</sub>P<sub>3</sub>).



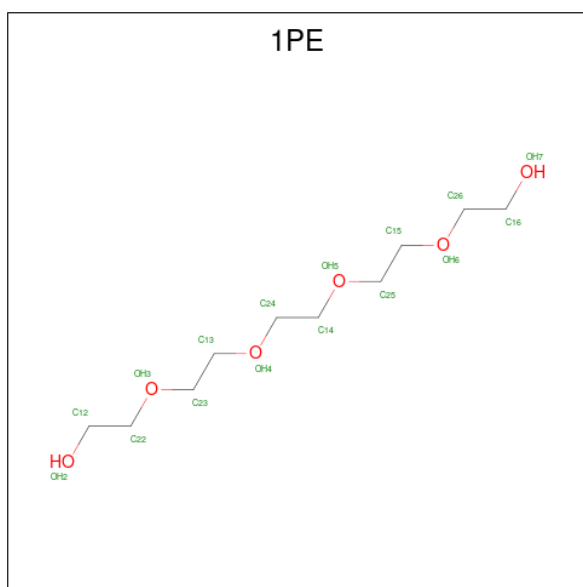
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	28	10	2	13	3	0	0

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	A	1	12	6	1	4	1	0	0

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	C O	0	0
			16	10 6		

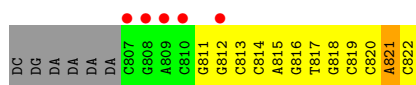
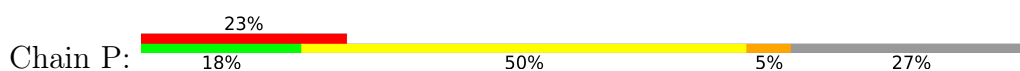
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	P	21	Total	O	0	0
			21	21		
10	T	42	Total	O	0	0
			42	42		
10	A	597	Total	O	0	0
			597	597		
10	B	56	Total	O	0	0
			56	56		

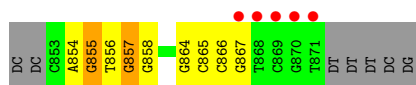
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

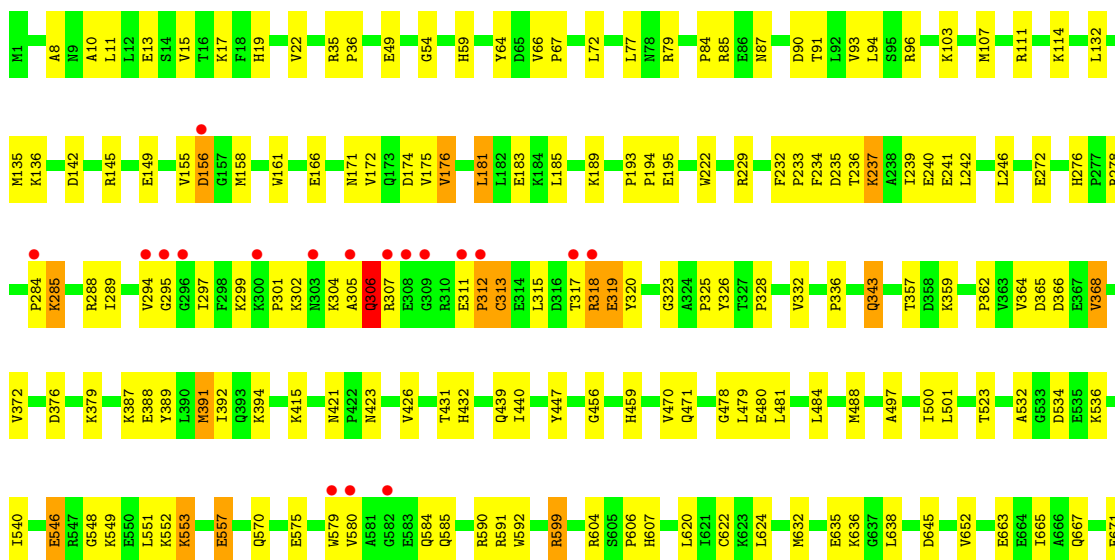
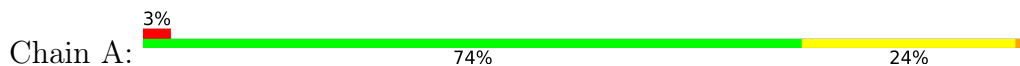
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*AP\*(DOC))-3')



- Molecule 2: DNA (5'-D(\*CP\*CP\*CP\*AP\*(8OG)P\*TP\*GP\*GP\*CP\*AP\*CP\*TP\*GP\*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*G)-3')

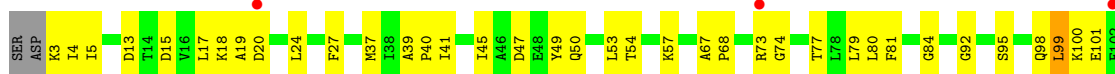


- Molecule 3: DNA polymerase





- Molecule 4: Thioredoxin 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.51Å 215.11Å 52.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.91 – 2.49 47.91 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.9 (47.91-2.49) 96.0 (47.91-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.80 (at 2.48Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.265 0.186 , 0.246	Depositor DCC
$R_{free}$ test set	1957 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtrriage
Anisotropy	0.344	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MES, 1PE, DOC, D3T, 8OG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	P	0.43	0/344	0.82	0/528
2	T	0.45	0/410	0.86	0/628
3	A	0.33	0/5671	0.57	1/7680 (0.0%)
4	B	0.30	0/817	0.57	0/1108
All	All	0.34	0/7242	0.60	1/9944 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
2	T	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	306	GLN	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	821	DA	Sidechain
2	T	857	DG	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	325	0	178	27	0
2	T	391	0	214	13	0
3	A	5534	0	5387	146	0
4	B	802	0	816	27	0
5	A	3	0	0	0	0
6	A	15	0	0	0	0
7	A	28	0	13	3	0
8	A	12	0	13	1	0
9	A	16	0	22	5	0
10	A	597	0	0	8	0
10	B	56	0	0	1	0
10	P	21	0	0	0	0
10	T	42	0	0	1	0
All	All	7842	0	6643	199	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:816:DG:H2''	1:P:817:DT:H5'	1.42	1.00
3:A:311:GLU:HB3	3:A:312:PRO:HD2	1.40	0.99
1:P:815:DA:H2''	1:P:816:DG:H5'	1.51	0.90
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.55	0.89
3:A:111:ARG:HH21	3:A:114:LYS:HD2	1.39	0.88
1:P:816:DG:H2''	1:P:817:DT:C5'	2.08	0.83
1:P:817:DT:H2''	1:P:818:DG:H5'	1.61	0.81
1:P:813:DC:H2''	1:P:814:DC:H5'	1.63	0.80
1:P:815:DA:H2''	1:P:816:DG:C5'	2.11	0.80
3:A:318:ARG:O	3:A:319:GLU:HB2	1.80	0.79
2:T:854:DA:H2''	2:T:855:8OG:H5'	1.66	0.78
3:A:570:GLN:HE22	3:A:606:PRO:HB3	1.48	0.77
4:B:45:ILE:HG13	4:B:99:LEU:HD13	1.66	0.75
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:111:ARG:NH2	3:A:114:LYS:HD2	2.05	0.71
3:A:391:MET:HE1	3:A:392:ILE:HD13	1.73	0.70
3:A:500:ILE:HG23	3:A:501:LEU:HD12	1.74	0.69
3:A:145:ARG:O	3:A:149:GLU:HG3	1.94	0.68
3:A:135:MET:HG3	3:A:174:ASP:OD1	1.93	0.68
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.76	0.67
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.76	0.67
4:B:73:ARG:HD2	4:B:73:ARG:O	1.94	0.67
3:A:311:GLU:HB3	3:A:312:PRO:CD	2.16	0.67
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.75	0.67
3:A:66:VAL:HB	3:A:67:PRO:HD3	1.78	0.66
3:A:570:GLN:NE2	3:A:606:PRO:HB3	2.11	0.66
3:A:534:ASP:CG	3:A:549:LYS:HG3	2.18	0.64
1:P:820:DC:H2''	1:P:821:DA:H5'	1.79	0.64
3:A:553:LYS:HB2	3:A:553:LYS:NZ	2.12	0.64
3:A:13:GLU:H	3:A:13:GLU:CD	2.01	0.63
4:B:3:LYS:HE2	4:B:50:GLN:NE2	2.13	0.63
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.81	0.62
3:A:391:MET:HE1	3:A:392:ILE:HA	1.81	0.62
2:T:858:DG:H4'	3:A:432:HIS:O	1.99	0.62
4:B:77:THR:HG22	4:B:79:LEU:HD13	1.82	0.61
1:P:819:DC:H1'	3:A:394:LYS:HE2	1.82	0.61
3:A:64:TYR:O	3:A:67:PRO:HD2	1.99	0.61
3:A:365:ASP:OD1	3:A:368:VAL:HG12	2.01	0.60
3:A:500:ILE:CG2	3:A:501:LEU:HD12	2.31	0.60
3:A:315:LEU:HD21	4:B:105:ALA:HB1	1.85	0.59
3:A:546:GLU:HA	3:A:546:GLU:OE1	2.03	0.58
2:T:854:DA:H2''	2:T:855:8OG:C5'	2.31	0.58
3:A:136:LYS:HD3	9:A:992:1PE:H162	1.84	0.58
3:A:284:PRO:HA	3:A:288:ARG:NH2	2.18	0.58
3:A:480:GLU:CD	7:A:823:D3T:H2'2	2.23	0.58
3:A:79:ARG:HD3	10:A:1070:HOH:O	2.03	0.58
1:P:813:DC:H1'	1:P:814:DC:H5''	1.85	0.58
3:A:388:GLU:O	3:A:392:ILE:HG12	2.03	0.58
3:A:667:GLN:O	3:A:671:GLU:HG3	2.04	0.58
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.04	0.58
3:A:553:LYS:O	3:A:557:GLU:HB2	2.03	0.58
3:A:678:ARG:NH1	3:A:691:ASP:OD1	2.37	0.57
1:P:817:DT:H2''	1:P:818:DG:C5'	2.32	0.57
2:T:864:DG:H2''	2:T:865:DC:O5'	2.06	0.56
3:A:302:LYS:H	3:A:306:GLN:NE2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:312:PRO:HG2	3:A:313:CYS:H	1.71	0.56
3:A:301:PRO:HA	3:A:306:GLN:NE2	2.21	0.56
3:A:312:PRO:O	3:A:313:CYS:CB	2.55	0.55
3:A:19:HIS:O	3:A:36:PRO:HD3	2.07	0.55
4:B:13:ASP:OD1	4:B:18:LYS:HE2	2.07	0.55
2:T:855:8OG:H2''	2:T:856:DT:H72	1.89	0.55
3:A:326:TYR:HB3	4:B:92:GLY:HA2	1.89	0.55
3:A:484:LEU:O	3:A:488:MET:HG2	2.06	0.54
3:A:17:LYS:HB3	3:A:17:LYS:NZ	2.23	0.54
3:A:478:GLY:HA2	7:A:823:D3T:O1B	2.07	0.54
4:B:4:ILE:HG21	4:B:57:LYS:HG3	1.89	0.54
3:A:323:GLY:O	3:A:325:PRO:HD3	2.08	0.54
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.90	0.53
3:A:312:PRO:O	3:A:313:CYS:HB2	2.08	0.53
1:P:816:DG:C2'	1:P:817:DT:C5'	2.85	0.53
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.43	0.53
3:A:301:PRO:HA	3:A:306:GLN:HE21	1.74	0.53
3:A:534:ASP:OD1	3:A:552:LYS:HE2	2.09	0.53
3:A:237:LYS:O	3:A:241:GLU:HG3	2.09	0.53
3:A:307:ARG:HB2	3:A:307:ARG:HH21	1.73	0.53
3:A:580:VAL:HG23	3:A:585:GLN:HG2	1.90	0.53
2:T:856:DT:C2'	2:T:857:DG:H5''	2.40	0.52
3:A:195:GLU:H	3:A:195:GLU:CD	2.11	0.52
4:B:67:ALA:HB3	4:B:68:PRO:HD3	1.91	0.52
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.44	0.52
3:A:233:PRO:HB2	3:A:456:GLY:O	2.09	0.52
1:P:813:DC:H2'	3:A:111:ARG:NH1	2.25	0.52
4:B:15:ASP:O	4:B:19:ALA:HB2	2.09	0.52
2:T:856:DT:H2''	2:T:857:DG:H5''	1.92	0.52
3:A:91:THR:HB	3:A:181:LEU:HD13	1.92	0.52
3:A:575:GLU:HG2	10:A:1552:HOH:O	2.10	0.52
3:A:579:TRP:HA	3:A:584:GLN:HA	1.91	0.52
3:A:189:LYS:HG2	3:A:194:PRO:HG3	1.92	0.51
3:A:376:ASP:OD2	3:A:379:LYS:HG3	2.09	0.51
1:P:817:DT:OP1	3:A:359:LYS:HB3	2.10	0.51
4:B:37:MET:O	4:B:40:PRO:HD2	2.11	0.51
3:A:107:MET:O	9:A:992:1PE:H161	2.11	0.51
3:A:304:LYS:O	3:A:305:ALA:HB3	2.10	0.51
3:A:497:ALA:O	3:A:501:LEU:HD13	2.10	0.51
1:P:813:DC:H2'	3:A:111:ARG:HH12	1.75	0.51
3:A:85:ARG:HD3	10:A:1059:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:172:VAL:O	3:A:176:VAL:HG12	2.11	0.51
1:P:820:DC:H5'	3:A:394:LYS:CE	2.41	0.50
1:P:816:DG:H1'	1:P:817:DT:H5''	1.93	0.50
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.11	0.50
3:A:423:ASN:OD1	3:A:599:ARG:NH2	2.45	0.50
1:P:813:DC:H2''	1:P:814:DC:C5'	2.38	0.49
3:A:272:GLU:O	3:A:288:ARG:HD3	2.11	0.49
3:A:299:LYS:HE2	10:A:1721:HOH:O	2.11	0.49
3:A:632:MET:O	3:A:636:LYS:HG3	2.12	0.49
3:A:368:VAL:O	3:A:372:VAL:HG23	2.11	0.49
3:A:276:HIS:HD2	3:A:278:ARG:H	1.60	0.49
3:A:359:LYS:O	3:A:359:LYS:HG2	2.12	0.49
1:P:820:DC:H2''	1:P:821:DA:C5'	2.43	0.48
3:A:305:ALA:O	3:A:311:GLU:HB2	2.12	0.48
1:P:821:DA:H5''	3:A:440:ILE:O	2.13	0.48
3:A:391:MET:HE3	3:A:447:TYR:CD2	2.49	0.48
3:A:183:GLU:HG2	10:A:1678:HOH:O	2.14	0.48
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.12	0.48
3:A:285:LYS:HE3	3:A:285:LYS:HA	1.96	0.48
3:A:136:LYS:HD2	9:A:992:1PE:H122	1.95	0.47
2:T:855:8OG:H2''	2:T:856:DT:C7	2.45	0.47
3:A:15:VAL:HG22	3:A:72:LEU:HD21	1.96	0.47
3:A:317:THR:O	3:A:318:ARG:O	2.31	0.47
3:A:8:ALA:HB3	3:A:64:TYR:OH	2.13	0.47
4:B:95:SER:OG	4:B:98:GLN:HG3	2.14	0.47
3:A:155:VAL:O	3:A:156:ASP:C	2.53	0.47
3:A:229:ARG:HD2	10:A:1022:HOH:O	2.15	0.47
1:P:814:DC:H2''	1:P:815:DA:C8	2.49	0.47
3:A:366:ASP:OD1	3:A:387:LYS:HD2	2.15	0.47
3:A:242:LEU:O	3:A:246:LEU:HG	2.15	0.47
1:P:811:DG:H2''	1:P:812:DG:C8	2.50	0.46
2:T:866:DC:H2''	2:T:867:DG:C8	2.50	0.46
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.82	0.46
4:B:27:PHE:CE1	4:B:79:LEU:HD22	2.51	0.46
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.50	0.46
2:T:854:DA:C2'	2:T:855:8OG:H5'	2.41	0.46
3:A:426:VAL:CG1	3:A:604:ARG:NH2	2.79	0.46
4:B:3:LYS:HE2	4:B:50:GLN:CD	2.35	0.46
3:A:632:MET:O	3:A:635:GLU:HG2	2.16	0.45
3:A:317:THR:O	3:A:318:ARG:C	2.54	0.45
3:A:698:PRO:CG	3:A:702:ILE:HD12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:357:THR:C	3:A:359:LYS:H	2.19	0.45
3:A:77:LEU:O	8:A:991:MES:H31	2.16	0.45
3:A:11:LEU:HD23	9:A:992:1PE:H221	1.98	0.45
3:A:158:MET:HA	3:A:161:TRP:CD2	2.51	0.45
3:A:235:ASP:HB2	3:A:459:HIS:CE1	2.52	0.45
3:A:236:THR:O	3:A:240:GLU:HG3	2.16	0.45
3:A:480:GLU:OE1	7:A:823:D3T:H2'2	2.18	0.44
3:A:84:PRO:HB2	3:A:87:ASN:OD1	2.17	0.44
1:P:813:DC:H1'	1:P:814:DC:C5'	2.48	0.44
3:A:59:HIS:CG	3:A:132:LEU:HD13	2.51	0.44
3:A:364:VAL:O	3:A:364:VAL:HG12	2.17	0.44
3:A:652:VAL:HG12	3:A:652:VAL:O	2.16	0.44
2:T:864:DG:H8	2:T:864:DG:H5'	1.82	0.44
3:A:10:ALA:C	9:A:992:1PE:H231	2.37	0.44
3:A:189:LYS:HE3	3:A:189:LYS:HB2	1.73	0.44
3:A:336:PRO:HB2	3:A:389:TYR:CE1	2.53	0.44
4:B:17:LEU:HA	4:B:84:GLY:HA2	1.99	0.44
1:P:815:DA:H2''	1:P:816:DG:H5''	1.96	0.44
3:A:294:VAL:HG12	3:A:295:GLY:N	2.33	0.44
3:A:320:TYR:OH	4:B:73:ARG:NH2	2.49	0.44
3:A:326:TYR:CE2	3:A:328:PRO:HG3	2.53	0.44
3:A:90:ASP:HB3	3:A:93:VAL:CG2	2.48	0.43
3:A:548:GLY:O	3:A:552:LYS:HG3	2.18	0.43
3:A:632:MET:HA	3:A:635:GLU:HG2	2.00	0.43
3:A:289:ILE:HD12	3:A:325:PRO:HB2	1.99	0.43
3:A:553:LYS:HB2	3:A:553:LYS:HZ2	1.80	0.43
3:A:663:GLU:O	3:A:696:MET:HE1	2.18	0.43
1:P:813:DC:C2'	1:P:814:DC:H5'	2.42	0.43
2:T:854:DA:O5'	3:A:532:ALA:HA	2.18	0.43
3:A:233:PRO:HA	3:A:415:LYS:HG2	2.00	0.43
4:B:13:ASP:HB3	10:B:1722:HOH:O	2.18	0.43
4:B:5:ILE:HD12	4:B:54:THR:HG21	2.00	0.43
3:A:590:ARG:HD2	3:A:592:TRP:O	2.20	0.42
4:B:24:LEU:HD22	4:B:103:LEU:HD21	2.01	0.42
4:B:79:LEU:HB3	4:B:81:PHE:CE1	2.54	0.42
10:T:1144:HOH:O	3:A:103:LYS:NZ	2.52	0.42
3:A:678:ARG:HD3	3:A:690:LEU:O	2.20	0.42
4:B:77:THR:CG2	4:B:79:LEU:HD13	2.46	0.42
3:A:536:LYS:O	3:A:540:ILE:HG13	2.20	0.42
3:A:579:TRP:CD1	3:A:584:GLN:HB2	2.55	0.42
4:B:41:ILE:O	4:B:45:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:8:ALA:HB1	3:A:15:VAL:CG2	2.50	0.42
3:A:591:ARG:O	3:A:591:ARG:HG2	2.20	0.42
1:P:821:DA:O4'	3:A:439:GLN:HA	2.19	0.41
3:A:276:HIS:CD2	3:A:278:ARG:H	2.37	0.41
3:A:470:VAL:HG12	3:A:471:GLN:N	2.35	0.41
3:A:22:VAL:HB	3:A:175:VAL:HG21	2.02	0.41
3:A:66:VAL:HG11	3:A:222:TRP:CH2	2.56	0.41
3:A:426:VAL:HG11	3:A:604:ARG:NH2	2.35	0.41
1:P:822:DOC:H5'	10:A:1507:HOH:O	2.21	0.41
3:A:90:ASP:HB3	3:A:93:VAL:HG23	2.02	0.41
3:A:96:ARG:NH1	10:A:1149:HOH:O	2.47	0.41
3:A:297:ILE:HB	4:B:101:GLU:OE1	2.21	0.41
3:A:391:MET:O	3:A:391:MET:HE2	2.20	0.41
4:B:74:GLY:O	4:B:77:THR:OG1	2.36	0.41
1:P:816:DG:C2'	1:P:817:DT:H5''	2.51	0.41
3:A:479:LEU:CD2	3:A:622:CYS:SG	3.09	0.41
3:A:481:LEU:HD23	3:A:481:LEU:HA	1.89	0.41
4:B:100:LYS:NZ	4:B:100:LYS:CB	2.84	0.41
2:T:855:8OG:OP1	3:A:607:HIS:ND1	2.45	0.40
3:A:676:ALA:O	3:A:680:VAL:HG23	2.21	0.40
4:B:49:TYR:HB3	4:B:53:LEU:HB3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	696/698 (100%)	658 (94%)	32 (5%)	6 (1%)	17	31
4	B	103/108 (95%)	98 (95%)	4 (4%)	1 (1%)	15	28
All	All	799/806 (99%)	756 (95%)	36 (4%)	7 (1%)	17	31



All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	306	GLN
3	A	318	ARG
3	A	319	GLU
3	A	313	CYS
4	B	20	ASP
3	A	312	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	570/579 (98%)	548 (96%)	22 (4%)	32 57
4	B	85/87 (98%)	82 (96%)	3 (4%)	36 62
All	All	655/666 (98%)	630 (96%)	25 (4%)	33 58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	142	ASP
3	A	166	GLU
3	A	171	ASN
3	A	176	VAL
3	A	181	LEU
3	A	232	PHE
3	A	237	LYS
3	A	285	LYS
3	A	306	GLN
3	A	332	VAL
3	A	343	GLN
3	A	368	VAL
3	A	391	MET
3	A	523	THR
3	A	546	GLU
3	A	551	LEU

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Mol	Chain	Res	Type
3	A	553	LYS
3	A	557	GLU
3	A	599	ARG
3	A	624	LEU
3	A	638	LEU
3	A	686	PHE
4	B	47	ASP
4	B	80	LEU
4	B	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	227	GLN
3	A	276	HIS
3	A	306	GLN
3	A	343	GLN
3	A	347	GLN
3	A	570	GLN
3	A	571	GLN
3	A	667	GLN
4	B	50	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	8OG	T	855	2,1	22,25,26	0.97	1 (4%)	30,37,40	1.76	5 (16%)
1	DOC	P	822	1,2	16,19,20	0.39	0	20,26,29	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8OG	T	855	2,1	-	1/7/21/22	0/3/3/3
1	DOC	P	822	1,2	-	0/7/18/19	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	855	8OG	C8-N7	-4.05	1.30	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	855	8OG	C2'-C1'-N9	-5.77	109.19	116.01
2	T	855	8OG	N7-C8-N9	4.97	112.48	106.58
2	T	855	8OG	C5-N7-C8	-3.30	104.72	109.47
2	T	855	8OG	O8-C8-N9	-2.65	122.29	125.99
2	T	855	8OG	C4-C5-N7	2.57	111.02	106.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	855	8OG	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	855	8OG	6	0
1	P	822	DOC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	A	904	-	4,4,4	0.27	0	6,6,6	0.07	0
8	MES	A	991	-	12,12,12	0.49	0	14,16,16	0.83	0
6	SO4	A	905	-	4,4,4	0.22	0	6,6,6	0.12	0
7	D3T	A	823	5	25,29,29	0.60	0	35,45,45	0.90	2 (5%)
9	1PE	A	992	-	15,15,15	0.87	0	14,14,14	0.87	0
6	SO4	A	906	-	4,4,4	0.26	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MES	A	991	-	-	3/6/14/14	0/1/1/1
7	D3T	A	823	5	-	2/22/31/31	0/2/2/2
9	1PE	A	992	-	-	5/13/13/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	823	D3T	O2G-PG-O1G	2.25	119.47	110.68
7	A	823	D3T	O3G-PG-O3B	-2.09	97.63	104.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

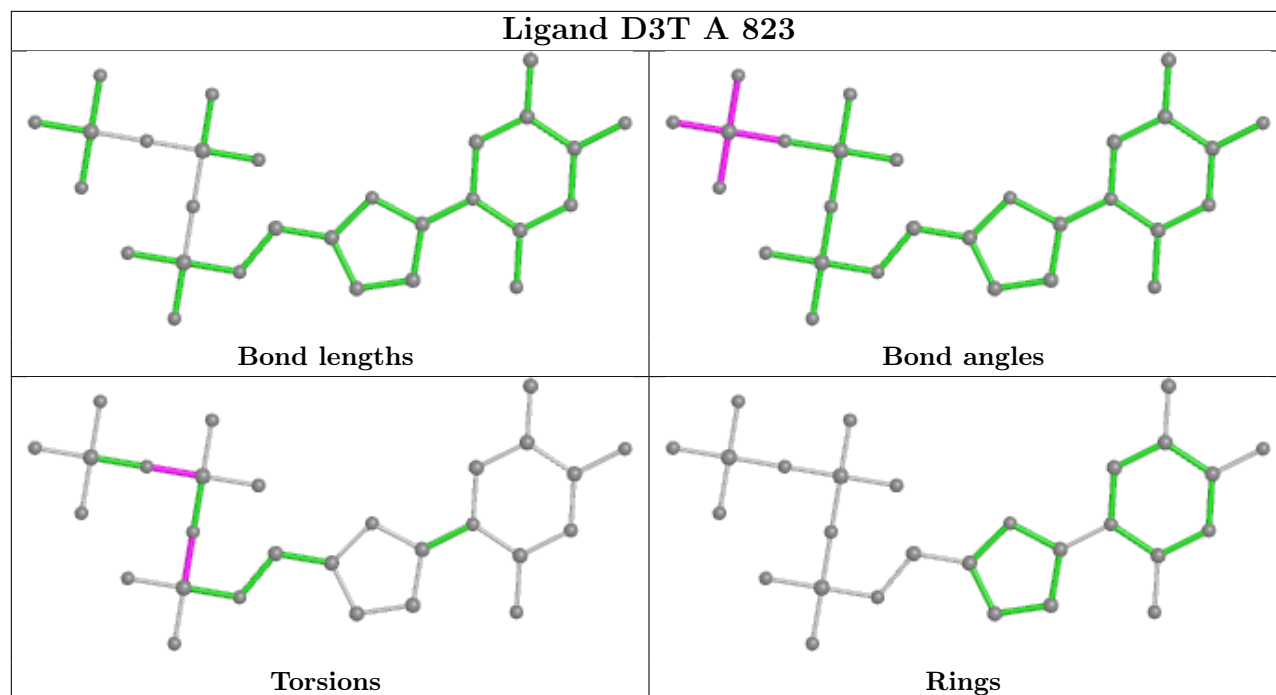
Mol	Chain	Res	Type	Atoms
8	A	991	MES	C7-C8-S-O2S
8	A	991	MES	C7-C8-S-O3S
9	A	992	1PE	OH7-C16-C26-OH6
9	A	992	1PE	OH2-C12-C22-OH3
7	A	823	D3T	PB-O3A-PA-O2A
8	A	991	MES	C7-C8-S-O1S
9	A	992	1PE	C25-C15-OH6-C26
7	A	823	D3T	PG-O3B-PB-O2B
9	A	992	1PE	C13-C23-OH3-C22
9	A	992	1PE	OH6-C15-C25-OH5

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	991	MES	1	0
7	A	823	D3T	3	0
9	A	992	1PE	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	P	15/22 (68%)	1.17	5 (33%) 0 0	19, 47, 100, 100	0
2	T	18/26 (69%)	0.92	5 (27%) 0 0	16, 33, 100, 100	0
3	A	698/698 (100%)	-0.13	18 (2%) 56 59	8, 22, 62, 89	0
4	B	105/108 (97%)	0.22	5 (4%) 30 32	17, 33, 54, 59	0
All	All	836/854 (97%)	-0.04	33 (3%) 39 42	8, 24, 64, 100	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	582	GLY	4.7
2	T	869	DC	4.5
1	P	807	DC	4.3
1	P	808	DG	4.2
2	T	870	DG	4.1
3	A	308	GLU	3.9
3	A	305	ALA	3.8
3	A	318	ARG	3.5
3	A	294	VAL	3.4
3	A	309	GLY	3.4
1	P	809	DA	3.2
4	B	107	LEU	3.2
3	A	579	TRP	3.2
3	A	317	THR	3.1
3	A	307	ARG	3.0
4	B	73	ARG	3.0
3	A	312	PRO	2.9
2	T	871	DT	2.9
3	A	156	ASP	2.8
3	A	296	GLY	2.8
3	A	303	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	810	DC	2.6
3	A	580	VAL	2.6
3	A	300	LYS	2.6
3	A	284	PRO	2.4
1	P	812	DG	2.3
2	T	868	DT	2.3
4	B	102	PHE	2.2
4	B	20	ASP	2.2
3	A	311	GLU	2.1
3	A	295	GLY	2.1
2	T	867	DG	2.1
4	B	106	ASN	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	8OG	T	855	23/24	0.94	0.16	19,23,32,35	0
1	DOC	P	822	18/19	0.98	0.15	12,15,16,17	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	A	901	1/1	0.79	0.09	24,24,24,24	0
9	1PE	A	992	16/16	0.86	0.26	37,43,50,51	0
5	MG	A	902	1/1	0.87	0.11	37,37,37,37	0
6	SO4	A	906	5/5	0.94	0.14	87,88,88,88	0

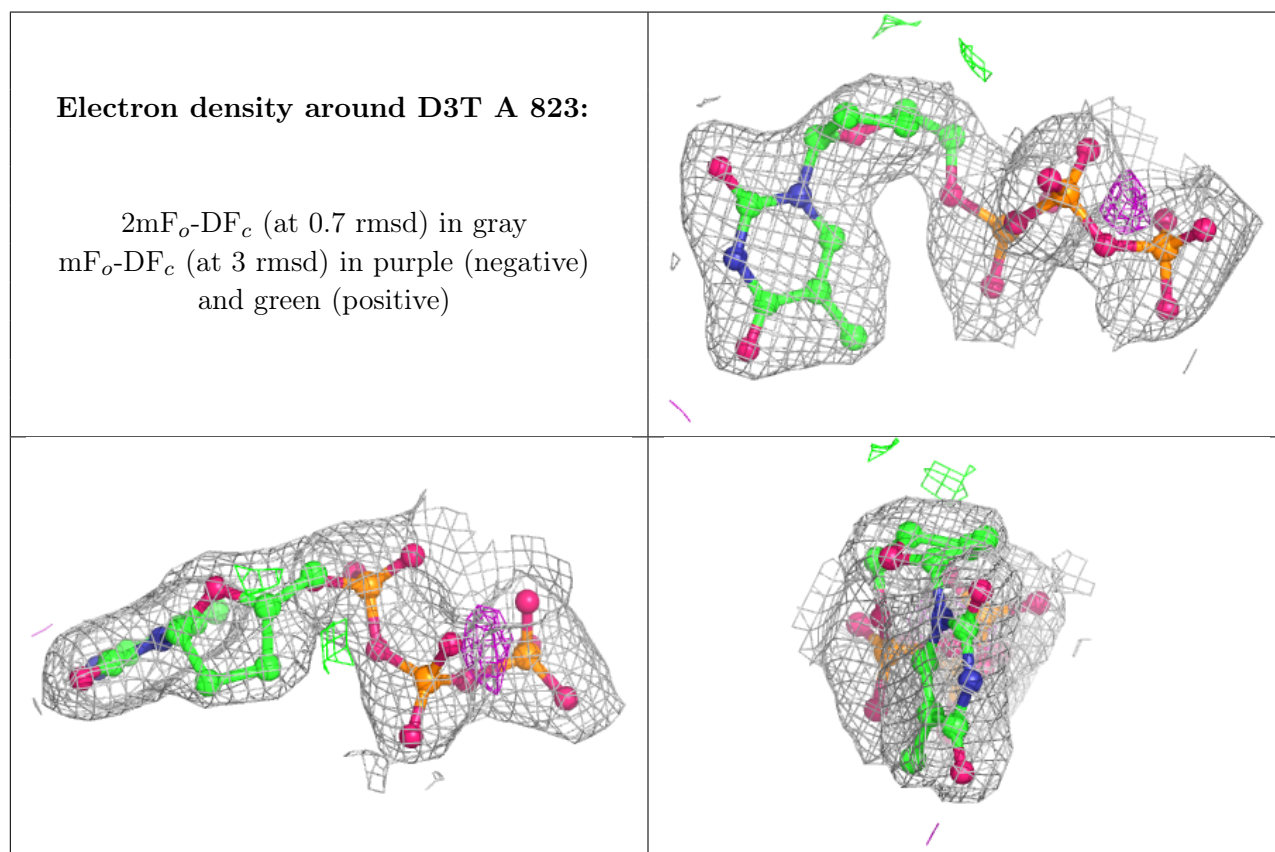
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	904	5/5	0.95	0.17	53,54,55,55	0
7	D3T	A	823	28/28	0.96	0.13	23,26,29,30	0
8	MES	A	991	12/12	0.97	0.16	39,42,44,44	0
6	SO4	A	905	5/5	0.97	0.18	58,58,59,59	0
5	MG	A	903	1/1	0.98	0.07	18,18,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.